

The inelastic hard dimer gas: a non-spherical model for granular matter.

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Abstract

We study a two-dimensional gas of inelastic smooth hard dimers. Since the collisions between dimers are dissipative, being characterized by a coefficient of restitution $\alpha < 1$, and no external driving force is present, the energy of the system decreases in time and no stationary state is achieved. However, the resulting non equilibrium state of the system displays several interesting properties in close analogy with systems of inelastic hard spheres, whose relaxational dynamics has been thoroughly explored.

We generalise to inelastic systems a recently method introduced [G.Ciccotti and G.Kalibaeva, J. Stat. Phys. **115**, 701 (2004)] to study the dynamics of rigid elastic bodies made up of different spheres hold together by rigid bonds. Each dimer consists of two hard disks of diameter d , whose centers are separated by a fixed distance a . By describing the rigid bonds by means of holonomic constraints and deriving the appropriate collision rules between dimers, we reduce the dynamics to a set of equations which can be solved by means of event driven simulation. After deriving the algorithm we study the decay of the total kinetic energy, and of the ratio between the rotational and the translational kinetic energy of inelastic dimers. We show numerically that the celebrated Haff's homogeneous cooling law t^{-2} , describing how the kinetic energy of an inelastic hard sphere system with constant coefficient of restitution decreases in time, holds even in the case of these non spherical particles. We fully characterize this homogeneous decay process in terms of appropriate decay constants and confirm numerically the scaling behavior of the velocity distributions.

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I. INTRODUCTION

Over the past two decades much progress has been made in understanding the dynamics of granular matter, i.e a collection of macroscopic particles interacting via a short range repulsive potential in which energy is lost in inelastic collisions^{1,2,3}. The industrial and technological importance of products which are either powders or granulates is now becoming generally recognized. Such a continued interest has unveiled a series of surprising phenomena and determined new challenges to physicists, because of the simultaneous presence of many body effects and non thermal fluctuations. In fact, in granular materials such as sand, cereals, steel balls etc. the ordinary temperature is irrelevant and consequently thermal equilibrium is not realized. Due to inelastic collisions a granular system, when not driven cools, i.e. the one particle velocity distribution tends to narrow in time^{4,5}. The inelastic hard sphere (IHS) model represents, perhaps, the simplest description of a granular system and most of the theoretical investigations are based on it. A collection of IHS sufficiently rarefied is called granular gas, because its dynamics consists of ballistic motions alternated with instantaneous binary collisions which conserve total momentum. The inelastic collisions are modeled by means of constant coefficient of normal restitution α , which determines the rate at which the kinetic energy is dissipated. Therefore, we possess nowadays a large amount of information concerning the IHS which has become the standard reference model for granular matter^{6,7,8,9,10,11,12}.

A natural question to ask is whether the behaviors observed in the IHS are generic or peculiar. The relevance of such an issue is not academic, since many actual materials, such as rice, needles, are far from being spherical but are elongated. As far as thermal systems are concerned the role of the shape of the constituent molecules in determining their thermodynamic behavior has been recognized since the pioneering work of Onsager¹³. Entropic effects (packing) of sufficiently anisotropic molecules (prolate ellipsoids, needles, spherocylinders, disks) determine the formation of mesophases¹⁴. In granular matter, instead, the effect of the non spherical shape of the particles is still largely unexplored in spite of its potential relevance in many phenomena such as nematic ordering transitions or violations of the energy equipartition. Few exceptions to such a trend are represented by the investigations of refs.^{15,16,17,18}.

Since the computer simulation is a fundamental tool in the study of granular systems, it

is crucial to devise an efficient method to treat the collisions, which usually represents the most time consuming part of a numerical code. The Event Driven (ED) method reduces such an effort to the calculation of the collision times, since the interactions in hard core systems occur only at the moment of collision. Once the shortest collision time has been computed all the particle positions are propagated inertially with the new velocities determined by the collision rules. The advantage over the fixed time step method in the case of hard objects is clear since there is no algorithmic error in the integration of the equations of motion. However, in the case of non spherical bodies the calculation of the collision time is not simple. Therefore, some authors resorted to a fixed time step method. Recently, Ciccotti and Kalibaeva¹⁹ have shown that it is possible to include a constraint, such as a fixed bond length between two elastic hard spheres, and preserve the advantages of the ED simulation. Hereafter we illustrate how to extend the ED method to a model of bond constrained inelastic hard disks.

The structure of the paper is the following. In section II we define the model and derive the equations of motion for a pure system of inelastic dimers. We also generalise the method to mixtures of inelastic dimers and disks and to systems of dimers in the presence of a fixed impenetrable wall. In section III we present numerical results obtained by means of the ED simulation. We discuss the properties of the homogeneous cooling state of inelastic hard dimers and obtain numerically the relevant parameters and the distribution functions. In section IV we draw the conclusions and discuss the future developments.

II. MODEL AND ALGORITHMS

In the present paper we discuss the properties of a system comprised of N dimers consisting of two identical hard disks of mass m rigidly connected. The diameter of the disks is d and the distance between their centers is a . In Fig. 1 there is a snapshot of the system. By describing the rigid bond between the two disks via an holonomic constraint¹⁹ we are able to apply the ED numerical simulation technique.

Let us consider the two-dimensional motion of an assembly of rigid dimers. We make the assumption of rigid body dynamics:

- The duration of contact is negligible and the interaction forces are high, so the velocity changes are nearly instantaneous without notable change in positions.

- The contact area is also negligible and the deformations are small in the impact zone so that the impact occurs at a single point of each body.
- Double contacts cannot occur simultaneously.

The motion of each dimer, A , is described by the velocity of its center of mass \mathbf{V}_A and by its angular velocity ω_A . The discontinuities of linear and angular momentum occurring at a collision event are obtained by imposing the conservation of the total linear and angular momentum and the law governing energy loss.

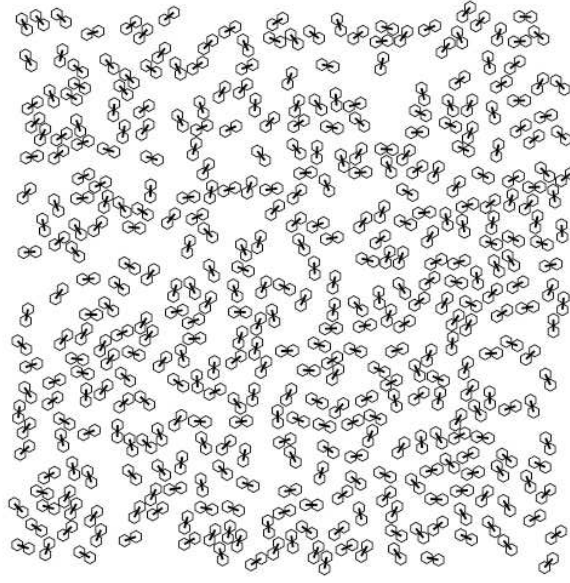


FIG. 1: Snapshot of a system of 400 dimers with $a = d$ and $\alpha = 0.95$.

A. Free streaming

In between collisions the dimers in the absence of external forces perform an unperturbed roto-translational motion. As shown in ref.¹⁹ such a free streaming can be described by the following parametric equations for the coordinates $\mathbf{r}_1(t)$ and $\mathbf{r}_2(t)$ of the centers of the two disks forming the dimer:

$$\begin{aligned} \mathbf{r}_1(t) &= \mathbf{R}_A(0) + \mathbf{V}_A(0)t - \frac{1}{2} \left[\mathbf{r}_2(0) - \mathbf{r}_1(0) \right] \cos(\omega_A t) - \frac{\mathbf{v}_2(0) - \mathbf{v}_1(0)}{2\omega_A} \sin(\omega_A t) \\ \mathbf{r}_2(t) &= \mathbf{R}_A(0) + \mathbf{V}_A(0)t + \frac{1}{2} \left[\mathbf{r}_2(0) - \mathbf{r}_1(0) \right] \cos(\omega_A t) + \frac{\mathbf{v}_2(0) - \mathbf{v}_1(0)}{2\omega_A} \sin(\omega_A t) \end{aligned} \quad (1)$$

where $\mathbf{R}_A(0)$ e $\mathbf{V}_A(0)$ are respectively the position and the velocity of the center of mass of the dimer A at the instant $t = 0$. The first two terms describe the translational motion, while the two last describe the rotational motion about the center of mass of the dimer. The angular velocity ω_A is obtained by solving the dynamics in the presence of the holonomic constraint

$$\chi = [\mathbf{r}_2(t) - \mathbf{r}_1(t)]^2 - a^2 = 0 \quad (2)$$

In fact differentiating with respect to t eq. (2) we obtain:

$$\begin{aligned} [\mathbf{v}_2(t) - \mathbf{v}_1(t)] \cdot [\mathbf{r}_2(t) - \mathbf{r}_1(t)] &= -\omega_A \left\{ [\mathbf{r}_2(0) - \mathbf{r}_1(0)] \sin(\omega_A t) - [\mathbf{v}_2(0) - \mathbf{v}_1(0)] \frac{\cos(\omega_A t)}{\omega_A} \right\} \\ &\cdot \left\{ [\mathbf{r}_2(0) - \mathbf{r}_1(0)] \cos(\omega_A t) + [\mathbf{v}_2(0) - \mathbf{v}_1(0)] \frac{\sin(\omega_A t)}{\omega_A} \right\} = 0 \end{aligned} \quad (3)$$

Using eqs. (2) and (3) we obtain that angular velocity is constant and given by:

$$\omega_A = \sqrt{\frac{[\mathbf{v}_2(0) - \mathbf{v}_1(0)]^2}{a^2}} \quad (4)$$

B. Collision times

In order to give a self-contained account of the method we include the determination of the collision times following the presentation given in ref.¹⁹. The condition for the collision between two “molecules” A and B, formed by the four atoms 1, 2 and 3, 4, respectively are:

$$\begin{aligned} [\mathbf{r}_3(t) - \mathbf{r}_1(t)]^2 &= d^2 \\ [\mathbf{r}_3(t) - \mathbf{r}_2(t)]^2 &= d^2 \\ [\mathbf{r}_4(t) - \mathbf{r}_1(t)]^2 &= d^2 \\ [\mathbf{r}_4(t) - \mathbf{r}_2(t)]^2 &= d^2 \end{aligned} \quad (5)$$

Substituting the equations (1) for the position of each hard disk as a function of time in the collision conditions (5) we get a set of equations in t , from which we take the smallest one as the collision time of the two molecules.

B.1 Dynamics of Collisions

In each collision between two dimers four disks are involved, therefore we write the conservation laws for the total linear momentum

$$m(\mathbf{v}_{1f} + \mathbf{v}_{2f} + \mathbf{v}_{3f} + \mathbf{v}_{4f}) = m(\mathbf{v}_{1i} + \mathbf{v}_{2i} + \mathbf{v}_{3i} + \mathbf{v}_{4i}) \quad (6)$$

and for the total angular momentum

$$m(\mathbf{r}_1 \times \mathbf{v}_{1f} + \mathbf{r}_2 \times \mathbf{v}_{2f} + \mathbf{r}_3 \times \mathbf{v}_{3f} + \mathbf{r}_4 \times \mathbf{v}_{4f}) = m(\mathbf{r}_1 \times \mathbf{v}_{1i} + \mathbf{r}_2 \times \mathbf{v}_{2i} + \mathbf{r}_3 \times \mathbf{v}_{3i} + \mathbf{r}_4 \times \mathbf{v}_{4i}) \quad (7)$$

where the subscripts i and f indicate pre-collisional and post-collisional observable, respectively. Since the variables \mathbf{r}_j ($j = 1, 4$) do not change during the instantaneous collision, we do not need to distinguish between their pre-collisional and post-collisional value.

Upon differentiating the constraint (2) we obtain relations between the velocities of the particles belonging to the same dimer:

$$\begin{cases} (\mathbf{v}_{2i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{12} = 0 \\ (\mathbf{v}_{2f} - \mathbf{v}_{1f}) \cdot \mathbf{r}_{12} = 0 \\ (\mathbf{v}_{4i} - \mathbf{v}_{3i}) \cdot \mathbf{r}_{34} = 0 \\ (\mathbf{v}_{4f} - \mathbf{v}_{3f}) \cdot \mathbf{r}_{34} = 0 \end{cases} \quad (8)$$

with $\mathbf{r}_{jk} \equiv \mathbf{r}_j - \mathbf{r}_k$. We simply satisfy eq. (6) by writing the change of momenta of the two molecules A and B with the help of a vector $\Delta\mathbf{v}$, to be specified in the following

$$\begin{cases} m(\mathbf{v}_{1f} + \mathbf{v}_{2f}) = m(\mathbf{v}_{1i} + \mathbf{v}_{2i}) + m\Delta\mathbf{v} \\ m(\mathbf{v}_{3f} + \mathbf{v}_{4f}) = m(\mathbf{v}_{3i} + \mathbf{v}_{4i}) - m\Delta\mathbf{v} \end{cases} \quad (9)$$

In order to satisfy simultaneously eq. (9) and the constraints (8) it has been shown, assuming that the colliding particles are 1 and 3, that one obtains the following expressions¹⁹

$$\begin{cases} \mathbf{v}_{1f} = \mathbf{v}_{1i} + \Delta\mathbf{v} - \frac{\Delta\mathbf{v} \cdot \mathbf{r}_{12}}{2a^2} \mathbf{r}_{12} \\ \mathbf{v}_{2f} = \mathbf{v}_{2i} + \frac{\Delta\mathbf{v} \cdot \mathbf{r}_{12}}{2a^2} \mathbf{r}_{12} \\ \mathbf{v}_{3f} = \mathbf{v}_{3i} - \Delta\mathbf{v} + \frac{\Delta\mathbf{v} \cdot \mathbf{r}_{34}}{2a^2} \mathbf{r}_{34} \\ \mathbf{v}_{4f} = \mathbf{v}_{4i} - \frac{\Delta\mathbf{v} \cdot \mathbf{r}_{34}}{2a^2} \mathbf{r}_{34} \end{cases} \quad (10)$$

The change of the angular momenta of the two colliding dimers are

$$\begin{cases} m(\mathbf{r}_1 \times \mathbf{v}_{1f} + \mathbf{r}_2 \times \mathbf{v}_{2f}) = m(\mathbf{r}_1 \times \mathbf{v}_{1i} + \mathbf{r}_2 \times \mathbf{v}_{2i}) + m\mathbf{r}_1 \times \Delta\mathbf{v} \\ m(\mathbf{r}_3 \times \mathbf{v}_{3f} + \mathbf{r}_4 \times \mathbf{v}_{4f}) = m(\mathbf{r}_3 \times \mathbf{v}_{3i} + \mathbf{r}_4 \times \mathbf{v}_{4i}) - m\mathbf{r}_3 \times \Delta\mathbf{v} \end{cases} \quad (11)$$

so that the conservation of the total angular momentum at collision implies that $\Delta\mathbf{v}$ is directed along the direction of the vector \mathbf{r}_{13} connecting the centers of the two colliding disks, i.e

$$\Delta\mathbf{v} = \Delta v \frac{\mathbf{r}_{13}}{d} \quad (12)$$

Finally substituting eq. (12) into eq. (10) we arrive at

$$\begin{cases} \mathbf{v}_{1f} = \mathbf{v}_{1i} + \Delta v \frac{\mathbf{r}_{13}}{d} - \Delta v \frac{\mathbf{r}_{13} \cdot \mathbf{r}_{12}}{2a^2d} \mathbf{r}_{12} \\ \mathbf{v}_{2f} = \mathbf{v}_{2i} + \Delta v \frac{\mathbf{r}_{13} \cdot \mathbf{r}_{12}}{2a^2d} \mathbf{r}_{12} \\ \mathbf{v}_{3f} = \mathbf{v}_{3i} - \Delta v \frac{\mathbf{r}_{13}}{d} + \Delta v \frac{\mathbf{r}_{13} \cdot \mathbf{r}_{34}}{2a^2d} \mathbf{r}_{34} \\ \mathbf{v}_{4f} = \mathbf{v}_{4i} - \Delta v \frac{\mathbf{r}_{13} \cdot \mathbf{r}_{34}}{2a^2d} \mathbf{r}_{34} \end{cases} \quad (13)$$

In order to fix the amplitude Δv we consider the change of total kinetic energy occurring in a single collision event:

$$\begin{aligned} \Delta E &= \frac{m}{2}(\mathbf{v}_{1f}^2 + \mathbf{v}_{2f}^2 + \mathbf{v}_{3f}^2 + \mathbf{v}_{4f}^2) - \frac{m}{2}(\mathbf{v}_{1i}^2 + \mathbf{v}_{2i}^2 + \mathbf{v}_{3i}^2 + \mathbf{v}_{4i}^2) = \\ &= m\Delta v^2 \left\{ 1 - \frac{1}{4a^2d^2} [(\mathbf{r}_{13} \cdot \mathbf{r}_{12})^2 + (\mathbf{r}_{13} \cdot \mathbf{r}_{34})^2] \right\} - \frac{m\Delta v}{d} (\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13} \end{aligned} \quad (14)$$

For a perfectly elastic collision the condition $\Delta E = 0$ determines Δv :

$$\Delta v = \frac{(\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13} / d}{1 - \frac{1}{4a^2d^2} [(\mathbf{r}_{13} \cdot \mathbf{r}_{12})^2 + (\mathbf{r}_{13} \cdot \mathbf{r}_{34})^2]} \quad (15)$$

To generalize the collision rule to the case of inelastic collisions we consider the variation of the relative velocity of the two colliding disks along the center to center direction:

$$(\mathbf{v}_{3f} - \mathbf{v}_{1f}) \cdot \mathbf{r}_{13} = (\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13} - 2\Delta v d \left\{ 1 - \frac{1}{4a^2d^2} [(\mathbf{r}_{13} \cdot \mathbf{r}_{12})^2 + (\mathbf{r}_{13} \cdot \mathbf{r}_{34})^2] \right\} \quad (16)$$

and impose the condition that the projection of the relative velocity along \mathbf{r}_{13} after the collision is proportional to the projection of the relative velocity before the collision via a coefficient of restitution α ($0 \leq \alpha \leq 1$), which takes into account the energy dissipation.

$$(\mathbf{v}_{3f} - \mathbf{v}_{1f}) \cdot \mathbf{r}_{13} = -\alpha (\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13} \quad (17)$$

In this case one sees that the rule (15) is modified

$$\Delta v = \frac{1 + \alpha}{2d} \frac{(\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13}}{1 - \frac{1}{4a^2d^2} [(\mathbf{r}_{13} \cdot \mathbf{r}_{12})^2 + (\mathbf{r}_{13} \cdot \mathbf{r}_{34})^2]} \quad (18)$$

By substituting the relation (18) into eq. (14) we find the corresponding energy loss in an inelastic collision

$$\Delta E = -m \frac{1 - \alpha^2}{4d^2} \frac{[(\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13}]^2}{1 - \frac{1}{4a^2d^2} [(\mathbf{r}_{13} \cdot \mathbf{r}_{12})^2 + (\mathbf{r}_{13} \cdot \mathbf{r}_{34})^2]} \quad (19)$$

Let us compare the energy dissipated (19) by two inelastic dimers with that associated with the collision of two inelastic hard disks of diameter d , mass m and coefficient of restitution α :

$$\Delta E_{dd} = -m \frac{1 - \alpha^2}{4d^2} [(\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13}]^2 \quad (20)$$

and notice that in the first case the amount dissipated depends on the relative orientation of the two dimers, the largest dissipation occurring for head to head collisions, where the two axes \mathbf{r}_{12} and \mathbf{r}_{34} are parallel to \mathbf{r}_{13} . This orientational dependence of the dissipation of dimers renders the model similar to a model of inelastic disks with a fluctuating coefficient of restitution.

B.2 Collision between a dimer and a disk

The behavior of mixtures of different grains is also a subject of extreme interest. The dimer-disk mixture has not been studied so far. It is a simple exercise to derive the collision rules in the case of the collision between a dimer and a hard disk having the same coefficient of restitution,

$$\begin{cases} \mathbf{v}_{1f} = \mathbf{v}_{1i} + \Delta \mathbf{u} - \frac{\Delta \mathbf{u} \cdot \mathbf{r}_{12}}{2a^2} \mathbf{r}_{12} \\ \mathbf{v}_{2f} = \mathbf{v}_{2i} + \frac{\Delta \mathbf{u} \cdot \mathbf{r}_{12}}{2a^2} \mathbf{r}_{12} \\ \mathbf{V}_{df} = \mathbf{V}_{di} - \frac{m}{M} \Delta \mathbf{u} \end{cases} \quad (21)$$

where we have assumed that the mass of the disk is M . \mathbf{R}_d is the position of disk center and σ its diameter. We also introduced the vector $\Delta \mathbf{u}$:

$$\Delta \mathbf{u} = (1 + \alpha_d) \frac{(\mathbf{V}_{di} - \mathbf{v}_{1i}) \cdot (\mathbf{R}_d - \mathbf{r}_1)}{1 + \frac{m}{M} - \frac{1}{2a^2C^2} [(\mathbf{R}_d - \mathbf{r}_1) \cdot \mathbf{r}_{12}]^2} \frac{(\mathbf{R}_d - \mathbf{r}_1)}{C^2} \quad (22)$$

with $C = (d + \sigma)/2$ and α_d is the coefficient of restitution.

In this case the total energy dissipation in a dimer-disk collision is

$$\Delta E_d = -m \frac{1 - \alpha_d^2}{2C^2} \frac{[(\mathbf{V}_{di} - \mathbf{v}_{1i}) \cdot (\mathbf{R}_d - \mathbf{r}_1)]^2}{1 + \frac{m}{M} - \frac{1}{2a^2 C^2} [(\mathbf{R}_d - \mathbf{r}_1) \cdot \mathbf{r}_{12}]^2} \quad (23)$$

B.3 Collision between a dimer and a smooth impenetrable wall

second extension of the previous methods concerns the collision of a dimer against an impenetrable hard wall with a restitution coefficient α_w . Taking the limits $\sigma \rightarrow \infty$, $M \rightarrow \infty$ and $\mathbf{V}_{di} = 0$, we find in this case:

$$\begin{cases} \mathbf{v}_{1f} = \mathbf{v}_{1i} + \Delta \mathbf{w} - \frac{\Delta \mathbf{w} \cdot \mathbf{r}_{12}}{2a^2} \mathbf{r}_{12} \\ \mathbf{v}_{2f} = \mathbf{v}_{2i} + \frac{\Delta \mathbf{w} \cdot \mathbf{r}_{12}}{2a^2} \mathbf{r}_{12} \end{cases} \quad (24)$$

with

$$\Delta \mathbf{w} = -(1 + \alpha_w) \frac{\mathbf{v}_{1i} \cdot \hat{\mathbf{n}}}{1 - \frac{1}{2a^2} (\hat{\mathbf{n}} \cdot \mathbf{r}_{12})^2} \hat{\mathbf{n}} \quad (25)$$

and $\hat{\mathbf{n}}$ is a unit vector normal to the surface of the wall.

The relative total energy change is

$$\Delta E_w = -m \frac{1 - \alpha_w^2}{2} \frac{(\mathbf{v}_{1i} \cdot \hat{\mathbf{n}})^2}{1 - \frac{1}{2a^2} (\hat{\mathbf{n}} \cdot \mathbf{r}_{12})^2} \quad (26)$$

III. COOLING DYNAMICS

In the present section we focus on the evolution of an initially homogeneous gas of inelastic ($\alpha < 1$) hard dimers constrained to move on a plane. The system consists of N particles contained in a square subject to periodic boundary conditions and is not externally driven. Inelastic collisions between the dimers result in a loss of kinetic energy and thus determine a “cooling” of the gas.

This problem has been attracting much interest since the inelastic collisions make the system to behave very different from standard molecular fluids and plays a central role in this sub-area of non equilibrium statistical mechanics. The discovery of the homogeneous cooling state (HCS), characterized by a one particle distribution function whose shape is self similar, if the velocity is appropriately rescaled, has triggered a lot of attention²⁰.

In order to put things in perspective we take as a reference system, a set of N inelastic hard disks of diameter σ in two spatial dimensions ($D = 2$), since its properties have been thoroughly studied. Such a system starting from an equilibrium state of a corresponding elastic hard disk system, cools down uniformly, and decreases its average kinetic energy per particle $E_{kin}(t) = \frac{D}{2} T(t)$ according to Haff's law⁴

$$T(t) = \frac{T_0}{(1 + \gamma\nu_0 t)^2} \quad (27)$$

where $T(t)$ is the so called granular temperature, T_0 the initial temperature, ν_0 is the equilibrium Enskog collision frequency at T_0 and the non dimensional parameter γ is:

$$\gamma = \frac{(1 - \alpha^2)}{2D}. \quad (28)$$

Remarkably the homogeneous cooling law holds in any spatial dimension, D , as far as smooth inelastic hard spheres are considered.

HCS is characterized by uniform density and velocity fields and is maintained only for a finite time, or for a finite number of collisions, since it is linearly unstable to fluctuations. After the initial homogeneous stage, the system enters an inhomogeneous cooling state where a vortex structure develops in the velocity field (shearing instability) followed by a density instability (clustering)^{5,21}.

A theoretical estimate of ν_0 for elastic hard disks is provided by the following Enskog expression

$$\nu_0 = 2\sqrt{\pi}n\sigma\sqrt{\frac{T_0}{m}}g(\sigma) \quad (29)$$

where n is the number of particles per unit area and $g(\sigma)$ is the hard disk equilibrium pair correlation function evaluated at contact¹⁷:

$$g(\sigma) = \frac{1 - \frac{7}{16}\eta}{(1 - \eta)^2} \quad (30)$$

and η is the area fraction $\eta = \pi n\sigma^2/4$. It is also useful, for future comparison, to express the number of atomic collisions per particle, τ , suffered by the particles until time t by the phenomenological relation connecting to the inelasticity parameter γ and the equilibrium collision frequency:

$$\tau(t) \equiv \frac{N_{atcoll}(t)}{N} = \frac{1}{\gamma} \ln(1 + \gamma\nu_0 t) \quad (31)$$

A second important property of the HCS concerns the velocity distribution function, which of course cannot be stationary due to the energy loss, but after a short transient assumes a form which depends on time only through the granular temperature, $T(t) = \frac{1}{2}mv_0^2(t)$,

$$f(\mathbf{v}, t) = \frac{n}{v_0(t)^D} \Phi\left(\frac{\mathbf{v}}{v_0(t)}\right) \quad (32)$$

with

$$v_0^2(t) = \frac{2}{Dn} \int d^D v \, \mathbf{v}^2 f(\mathbf{v}, t) \quad (33)$$

The scaling function, $\Phi(z)$ is time independent in the HCS and in the limit of small dissipation approaches a Gaussian, i.e. $\Phi(z) \simeq \pi^{-D/2} \exp(-z^2)$. For smaller values of α a perturbation theory about the elastic state accounts for the departure from the Maxwellian¹¹.

Is the scenario described above preserved in a gas of hard inelastic dimers? In other words can we find constant values γ^{eff} and ν_0^{eff} such that eqs. (27) and (31) still hold with these effective parameters? Secondly, do the distribution functions of the translational and rotational components have the scaling property (32)? If the answer is affirmative the inelastic hard dimer system possesses a homogeneous cooling state, whose importance for the study of granular gases has been stressed by various authors^{20,21,22,23,24,25}.

The evolution of the inelastic dimer system can be characterized in terms of the average values per particle of the total kinetic energy, the translational and the rotational kinetic energy. The last two quantities averaged over the particles define the partial granular temperatures:

$$T_{tr}(t) = \langle E_{tr}(t) \rangle = \frac{m}{N} \sum_{A=1}^N [\mathbf{V}_A(t) - \langle \mathbf{V}_A(t) \rangle]^2 \quad (34)$$

$$T_{rot}(t) = 2 \langle E_{rot}(t) \rangle = \frac{I}{N} \sum_{A=1}^N \omega_A^2(t) \quad (35)$$

where $\mathbf{V}_A(t)$ is the center of mass velocity of a single dimer A , ω_A its angular velocity and $I = ma^2/2$ its moment of inertia. Our results for the decay of the average total kinetic energy $E(t) = T_{tr}(t) + \frac{1}{2}T_{rot}(t)$ are shown Fig. 2. We observe that the cooling process occurs according to the same universal inverse power law t^{-2} which characterizes the inelastic hard sphere systems. In addition, when plotted as a function of the total number of atomic collisions suffered on the average by a dimer times the inelasticity parameter $(1 - \alpha^2)$, the

curves corresponding to different values of α nicely fall one onto the other. However, the slope characterizing the various dimer systems is different, being in fact slower, from the corresponding slope of the hard disk systems. This feature represents the fingerprint of the structure of the dimers.

A second remarkable feature is the validity of the logarithmic law (31) (see Fig. 3), with the effective parameters ν_0^{eff} and $\gamma^{eff} = (1 - \alpha^2)/(2D_e)$ shown in table I. Notice that $D_e = D$ in the case of inelastic D -dimensional smooth hard spheres. We note that while D_e is nearly independent of the elongation, a , of the dimer, the initial collision frequency ν_0^{eff} does depend on a , being connected with the total cross section of this object.

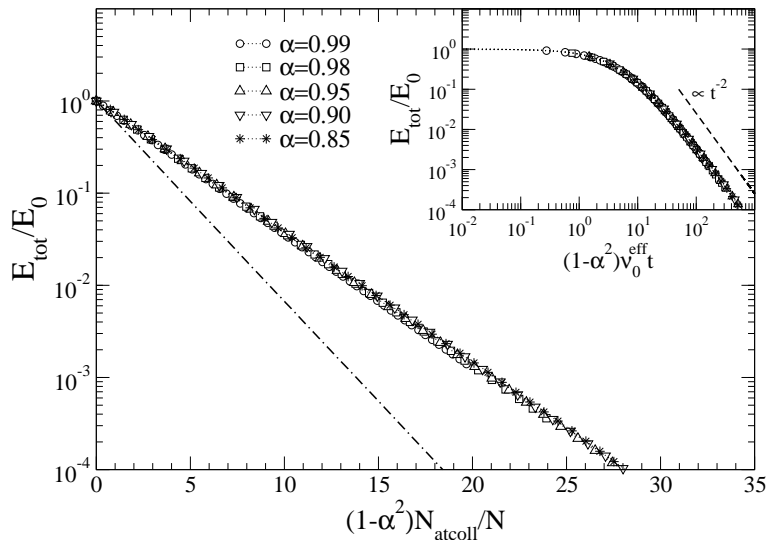


FIG. 2: Data collapse for dimers having different coefficients of restitution obtained by plotting the decay of total energy as a function of $(1 - \alpha^2)N_{atcoll}/N$, i.e. the total number of collisions suffered by a molecule multiplied by the inelasticity factor $(1 - \alpha^2)$. The dashed line corresponds to the energy decay of the reference hard disk system and shows a faster decay. In the inset the same quantities are shown as functions of the rescaled time $\nu_0^{eff}t$, showing the expected Haff's inverse power law decay.

The entries of table I have been obtained by fitting the numerical data with the logarithmic law eq. (31) with D_e and ν_0^{eff} used as fitting parameters. Our data analysis reveals that in all cases considered the fit is very good and that D_e is very close to 3.

We use a simple heuristic argument in order to derive the slower cooling rate of the hard dimers with respect to the disks. Let us compare formulae (19) and (20), representing

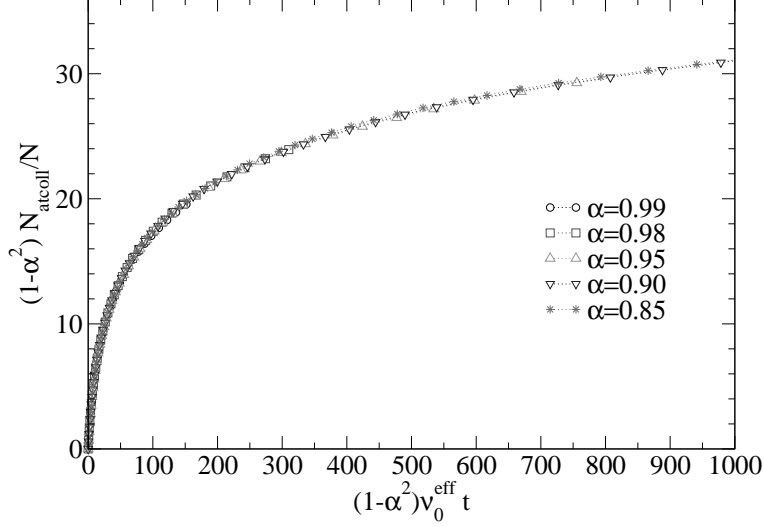


FIG. 3: Average number of atomic collisions per dimer rescaled by the inelasticity factor $(1-\alpha^2)$ as a function of the rescaled time $\nu_0^{eff}t$ for various values of the inelasticity and for a center-to-center distance $a = d$.

the energy dissipated in a collision between two dimers and two disks, respectively. What renders the behavior of the two systems different, when the coefficient of restitution α of both is the same, is the presence of the angular weighting factor, f :

$$f = \frac{1}{2 - \frac{1}{2a^2d^2} [(\mathbf{r}_{13} \cdot \mathbf{r}_{12})^2 + (\mathbf{r}_{13} \cdot \mathbf{r}_{34})^2]} \quad (36)$$

We can rewrite eq. (19) as

$$\Delta E = -m \frac{1-\alpha^2}{2d^2} f [(\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13}]^2 \quad (37)$$

We consider the average value of eq. (37) over many collisions, here indicated with the symbol $\langle \cdot \rangle$ and assume the following factorization

$$\langle \Delta E \rangle = -m \frac{1-\alpha^2}{2} \langle f \rangle \frac{1}{d^2} \langle [(\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13}]^2 \rangle \quad (38)$$

The last average turns out to be proportional to the average total energy, i.e.:

$$\frac{1}{d^2} \langle [(\mathbf{v}_{3i} - \mathbf{v}_{1i}) \cdot \mathbf{r}_{13}]^2 \rangle \simeq \frac{\langle E \rangle}{m} \quad (39)$$

which gives

$$\langle \Delta E \rangle = -\frac{1-\alpha^2}{2} \langle f \rangle \langle E \rangle. \quad (40)$$

We compute $\langle f \rangle$, assuming a dimer elongation $a = d$. It is straightforward to see that the angles formed by the directions \mathbf{r}_{13} and \mathbf{r}_{12} or \mathbf{r}_{34} are subjected to the constraint, required by the condition of non overlapping two dimers, that only the angles comprised between $-2\pi/3$ and $2\pi/3$ are allowed (see Fig. 4). We further assume a uniform distribution of these angles in the above interval, a guess which is confirmed numerically. As shown in Fig. 5, the computed distribution is almost uniform. Using this fact, we perform the average of formula (36) obtaining the value $\langle f \rangle = 0.64$. With this value we obtain the effective “dimension” $D_e = D/\langle f \rangle = 3.12$ which is compatible with the numerical values shown in table I. Intuitively this result is consistent with the idea that the energy stored in the rotational degree of freedom is only indirectly affected in the dissipation process and provides a kind of reservoir slowly dissipated.

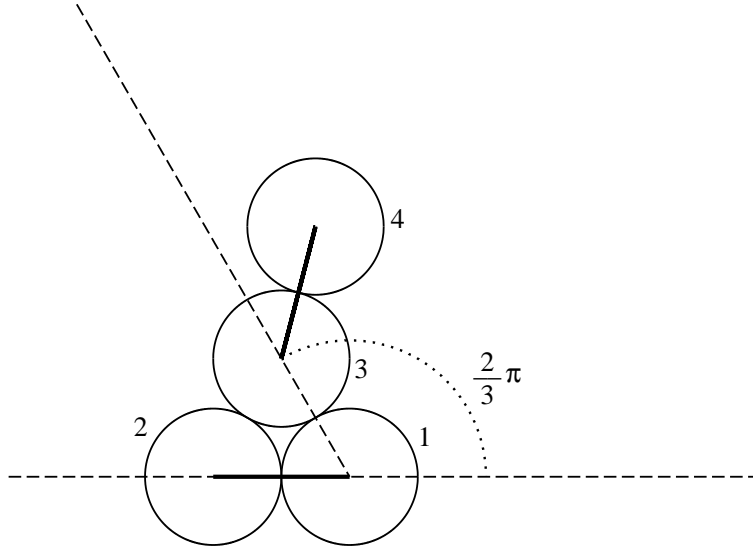


FIG. 4: Allowed angle between the directions \mathbf{r}_{13} and \mathbf{r}_{12} when two dimers are at contact. Since the dimers cannot overlap only the angles between $-2\pi/3$ and $2\pi/3$ are allowed.

A. Energy equipartition

One of the most peculiar features of granular systems is the lack of energy equipartition among different kinetic degrees of freedom. Such a phenomenon has been observed both in driven and undriven systems of smooth and rough hard-sphere mixtures^{26,27,28,29} and during the homogeneous cooling of a gas of inelastic needles¹⁵.

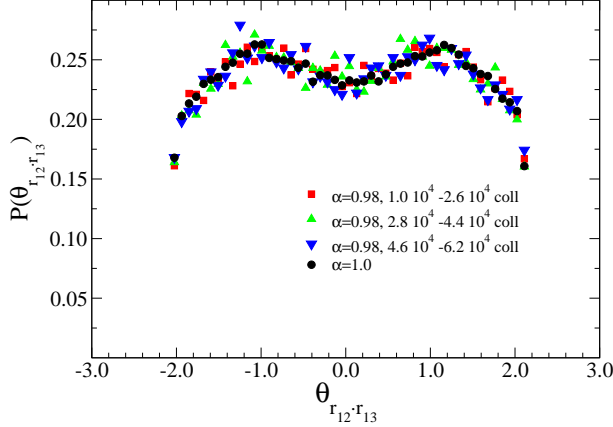


FIG. 5: Distribution of the angle between \mathbf{r}_{12} and \mathbf{r}_{13} measured in subsequent intervals, each containing 10^4 collisions. The distribution has been obtained for 900 dimers, $\alpha = 0.98$. The elastic case $\alpha = 1.0$ is also shown (bullets) for comparison.

In the case of dimers, the translational and rotational degrees of freedom satisfy the equipartition of energy only when $\alpha = 1$, as required by equilibrium statistical mechanics. We have evaluated numerically this property by fitting the time series for the ratio $K(\tau) = E_{tr}/E_{rot}$ by means of the linear least-square fit $\bar{K}(\tau) = a_0 + a_1\tau$. We have performed a t-Student statistical test of the data to determine the 99% confidence intervals for a_0 and a_1 ³¹. The result of such a test shows that a_1 is consistent with the value zero (see table II). As already established for mixture of inelastic hard spheres²⁸ the ratio K deviates from the corresponding elastic value ($K = 2$), but attains a constant ratio during the homogeneous cooling regime. We observe from table II that the larger the inelasticity the larger the breakdown of energy equipartition, and the longer the dimer the larger the deviation.

B. Velocity distribution functions

We turn now attention to the velocity distribution functions. As discussed above one of the characterizing features of the HCS is the existence of a time independent scaling function $\Phi(z)$. We have obtained numerically the related velocity distribution functions for the two translational components of the center of mass velocity and for the rotational velocity. These (normalized) distributions are displayed in Figs. 6 and compared with the Gaussian. We have not tried to measure departures from the Maxwellian, a task beyond the scope of the present work. Moreover, it is known from the literature^{11,30} that in the

case of inelastic hard-spheres these departures are small in the range $0.6 < \alpha < 1$ so that the Gaussian remains a valid approximation in the HCS of inelastic hard spheres. We guess from the present data that such a behavior remains true even in the case of the dimers.

To summarize there is evidence that inelastic hard dimers display a normal behavior in the HCS even with respect to the nature of their velocity distribution functions which are nearly Gaussian. Thus the analogy with the hard-sphere system is complete.

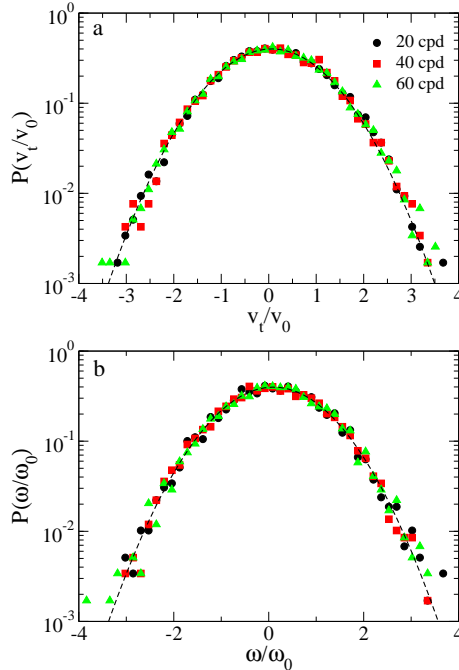


FIG. 6: a) Normalized translational velocity distribution function for dimers of elongation $a = d$ after different number of collisions per dimer (cpd). b) Normalized rotational velocity distribution functions for the same case. A gaussian curve (dashed line) is plotted for comparison.

IV. CONCLUSION AND OUTLOOK

We have investigated the dynamics of an undriven gas of inelastic hard dimers. The first achievement of this work has been to formulate properly the dynamics of pure inelastic dimer systems and that of a binary mixture of inelastic dimers and disks. Using such results we treated a pure gas of dimers with the ED algorithm. To validate the model and uncover some new physics we have then studied numerically the relaxation dynamics of such a system during the homogeneous cooling stage for various choices of the physical parameters. By

considering the total, translational and rotational kinetic energies of the dimers, we have found that their decay, following an initial short transient, agrees, as far as the system remains homogeneous, with the one observed in the case of a gas of IHS, that is Haff's cooling law. The different geometrical shape manifests itself in determining an identical pattern of cooling, although with a slower cooling rate which is related with the internal structure of the dimers. Moreover, we have found that the energy equipartition principle does not hold, although the ratio between rotational and translational energy is constant and almost equal to the equipartition value.

The one-particle velocity distribution functions of the system remain always close to the Maxwellian with properly scaled parameters both in the case of the center of mass translational and rotational degrees of freedom. These observations allow us to conclude that a HCS exists also in the case of inelastic hard dimers.

Preliminary work has also indicated interesting trends in the stages following the homogeneous cooling regime, in particular we have observed that on a longer time scale the system breaks its homogeneity showing vortex structures in the velocity field (shearing instability) and clustering. Both phenomena have a counterpart in systems of spherically symmetric particles. However, a careful analysis of these results requires further work.

V. ACKNOWLEDGMENTS

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TABLE I: Dependence of the parameters D_e and ν_0^{eff}/ν_0 on the coefficient of restitution and on the elongation of the dimer. For comparison the hard disk theoretical values are $D_e = 2$ and as a numerical check we applied the same procedure as in the case of dimers and obtained $D_e = 1.998$ at area fraction $\pi n \sigma^2/4 = 5.7 \times 10^{-4}$.

	α	D_e	ν_0^{eff}/ν_0
$a/d = 0.5$	0.99	3.003	1.07
	0.98	3.013	1.08
	0.95	3.028	1.08
	0.90	3.079	1.11
	0.85	3.109	1.13
$a/d = 1.0$	0.99	2.987	1.26
	0.98	3.014	1.25
	0.95	3.038	1.28
	0.90	3.086	1.32
	0.85	3.041	1.31
$a/d = 1.5$	0.99	3.004	1.45
	0.98	3.031	1.47
	0.95	3.059	1.50
	0.90	3.050	1.48
	0.85	3.102	1.50

TABLE II: Dependence of the ratio K between translational and rotational energy, on coefficient of restitution and elongation. The values Δa_0 and Δa_1 , concerning the 99% confidence intervals $a_0 \pm \Delta a_0$ and $a_1 \pm \Delta a_1$, are also shown.

	α	a_0	Δa_0	a_1	Δa_1
$a/d = 0.5$	1.0	1.999	1×10^{-3}	-2.86×10^{-6}	1.2×10^{-6}
	0.98	2.014	1×10^{-3}	-2.82×10^{-5}	3.5×10^{-6}
	0.95	1.994	2×10^{-3}	6.83×10^{-5}	1.0×10^{-5}
	0.85	2.056	2×10^{-3}	2.17×10^{-4}	1.5×10^{-5}
$a/d = 1.0$	1.0	2.001	1×10^{-3}	1.35×10^{-5}	2.1×10^{-6}
	0.98	1.989	1×10^{-3}	4.84×10^{-5}	3.1×10^{-6}
	0.95	2.046	1×10^{-3}	-2.50×10^{-4}	8.6×10^{-6}
	0.85	2.064	2×10^{-3}	-4.78×10^{-5}	1.7×10^{-5}
$a/d = 1.5$	1.0	1.987	1×10^{-3}	3.22×10^{-5}	2.0×10^{-6}
	0.98	2.025	1×10^{-3}	-5.38×10^{-5}	3.3×10^{-6}
	0.95	2.036	2×10^{-3}	-1.13×10^{-4}	9.2×10^{-6}
	0.85	2.075	2×10^{-3}	2.06×10^{-4}	1.6×10^{-5}